

Complementarity and correlations

Lorenzo Maccone¹, Dagmar Bruß², Chiara Macchiavello¹

¹*Dip. Fisica and INFN Sez. Pavia, University of Pavia, via Bassi 6, I-27100 Pavia, Italy*

²*Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany*

We provide an interpretation of entanglement based on classical correlations between measurement outcomes of complementary properties: states that have correlations beyond a certain threshold are entangled. The reverse is not true, however. We also show that, surprisingly, all separable nonclassical states exhibit smaller correlations for complementary observables than some strictly classical states. We use mutual information as a measure of classical correlations, but we conjecture that the first result holds also for other measures (e.g. the Pearson correlation coefficient or the sum of conditional probabilities).

PACS numbers: 03.65.Ud, 03.65.Ta, 03.67.Ac, 03.67.Hk

Two properties of a quantum state are called complementary if they are such that, if one knows the value of one property, all possible values of the other property are equiprobable. More rigorously, let $|a_i\rangle$ represent the eigenstates corresponding to possible values of a nondegenerate property $A = \sum_i f(a_i)|a_i\rangle\langle a_i|$, and $|c_j\rangle$ the eigenstates of a nondegenerate property $C = \sum_j g(c_j)|c_j\rangle\langle c_j|$ (with f and g arbitrary bijective functions). Then A and B are complementary properties if for all i, j we have $|\langle a_i|c_j\rangle|^2 = 1/d$, d being the Hilbert space dimension. Clearly complementary properties with this definition identify two mutually unbiased bases (MUBs) [1]. Here we study what classical correlations in the measurements of these complementary properties tell us about the quantum correlations of the state of the system.

Typically one discusses entanglement [2] in terms of non-locality, Bell inequality violations, monotones over LOCC, etc. For example, previous literature on entanglement focused on time-reversal (for the PPT criterion [3, 4]), local uncertainty relations [5–9], entropic uncertainty relations [10–13], entanglement witnesses [14–17], concurrence [18], the cross-norm criterion [19] and the covariance matrix criterion [20–24] (the latter encompassing many of the former). In contrast to these studies, we focus specifically on classical correlations for complementary properties. Classical correlations are typically quantified in terms of the mutual information, which is the main quantity considered here. We will also discuss the case of alternative measures such as the Pearson correlations and the sum of conditional probabilities. In [25] related approaches using specific measures of correlations (different from the ones used here) were proposed.

The outline of the paper follows. We start by describing the general scenario we employ for correlation evaluation. We then introduce different measures of correlations and state our results and our conjectures regarding entanglement and quantum correlations. We provide some examples of applications. The details of the proofs of our results are reported in the supplemental material.

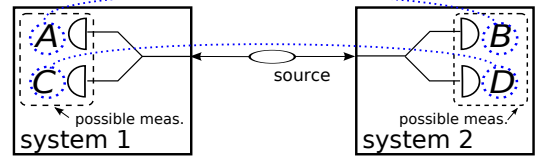


FIG. 1: Complementary correlation measurements. Each of two systems is subject to the measurement of one of two observables: either A or C on system 1 and either B or D on system 2. Correlations are evaluated between the results of A and B and between C and D (dashed lines). A and C are complementary on the first system, B and D on the second.

Complementary correlations:— Consider two systems of finite dimension d ([44]) and two observables $A \otimes B$ and $C \otimes D$ (Fig. 1) where A and C are complementary on the first system (namely $|\langle a_i|c_j\rangle| = 1/\sqrt{d}$ for all eigenstates of A and C) and B and D on the second. For example, take the computational basis of the two systems as the eigenstates of A and B , and the Fourier basis as the ones of C and D . We can quantify the correlations between the results of measurements of A and B with some correlation measure \mathcal{X}_{AB} and the correlations between C and D with \mathcal{X}_{CD} . As \mathcal{X} below we will define and investigate three possibilities: the mutual information $\mathcal{X}_{XY} = I_{XY}$, the sum of conditional probabilities $\mathcal{X}_{XY} = S_{XY}$, and the Pearson correlation coefficient $\mathcal{X}_{XY} = C_{XY}$. A measure of the overall correlation of the initial state, which we name the “complementary correlations”, can then be given as the sum of the absolute value of the two measures $|\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|$ or as the product $|\mathcal{X}_{AB}\mathcal{X}_{CD}|$. The latter is typically a weaker measure than the former, since an upper bound for the sum implies an upper bound for the product. Indeed, $(|\mathcal{X}_{AB}|^{1/2} - |\mathcal{X}_{CD}|^{1/2})^2 \geq 0$ implies $2\sqrt{|\mathcal{X}_{AB}\mathcal{X}_{CD}|} \leq |\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|$. Thus we will mainly consider the sum of correlations for complementary observables $|\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|$ as a way to evaluate the complementary correlations.

Mutual Information:— We start considering the mutual information: $I_{AB} \equiv H(A) - H(A|B)$, where $H(A)$

is the Shannon entropy of the probabilities of the measurement outcomes of the first system and $H(A|B)$ is the conditional entropy of the outcomes of the first conditioned on the second. The complementary correlations are then $I_{AB} + I_{CD}$.

The relation of this quantity to the entanglement and the discord of the state of the system is illustrated by the following results: (i) The state of a bipartite composite quantum system is maximally entangled if and only if there exist two complementary measurement bases where $I_{AB} + I_{CD} = 2 \log_2 d$; (ii) If

$$I_{AB} + I_{CD} > \log_2 d, \quad (1)$$

the state of the bipartite system is entangled (see also [26]); (iii) The separable states that satisfy this inequality with equality (i.e. $I_{AB} + I_{CD} = \log_2 d$), are the classically-correlated (CC) zero-discord states of the form

$$\rho_{cc} = \sum_i |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|/d \quad (2)$$

with $|a_i\rangle$ and $|b_i\rangle$ eigenstates of A and B (or the analogous state with a uniform convex combination of eigenstates of C and D). Some examples of $I_{AB} + I_{CD}$ for various families of states are plotted in Fig. 2a, where we emphasize the threshold $\log_2 d$ above which all states are entangled.

The first result follows from the fact that each term in the sum is upper bounded by $\log_2 d$ by definition. The maximum value for the sum is then $2 \log_2 d$ and is achievable if and only if there is maximal correlation both between A and B , and between C and D . Simple properties of the conditional probabilities (see supplemental material) imply that this can happen for a suitable choice of observables if and only if the state is maximally entangled. The second result is a consequence of the concavity of the entropy and of Maassen and Uffink's entropic uncertainty relation [27] (see supplemental material for the details). It gives a sufficient condition for entanglement that can be used for entanglement detection. The third result is surprising: one might expect that the separable states at the boundary with the entangled region are highly quantum correlated, whereas we find that they only have classical correlations (CC) and no discord. This means that quantum correlated states without entanglement do not have higher correlations for complementary properties than CC states. This result is peculiar for the mutual information as a figure of merit, it is no longer true for the Pearson correlation (where a family of QQ states sits on the border, as shown in Fig. 2b). It can be proved by analyzing the conditions for equality of the concavity of the entropy and of Maassen and Uffink's inequality (see supplemental material).

Pearson correlation:— The second measure of correlation we consider is the Pearson correlation coefficient

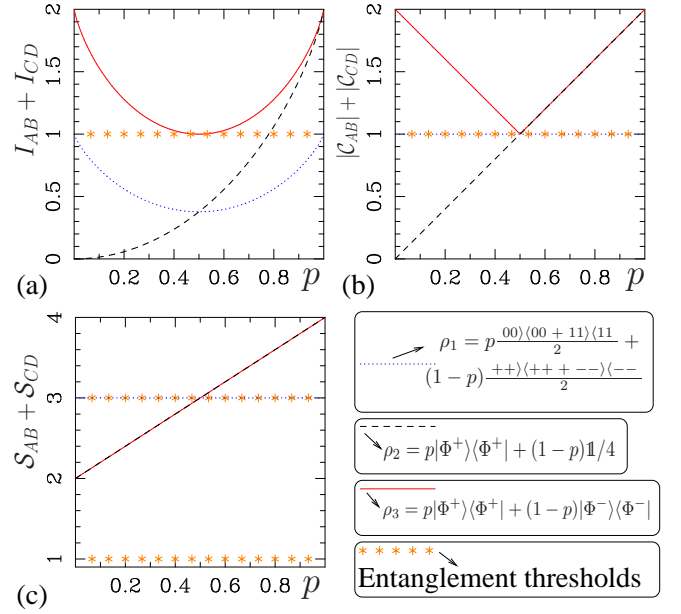


FIG. 2: Examples of complementary correlations for different measures of correlation and different families of states. (a) Correlation $I_{AB} + I_{CD}$ plotted as a function of the parameter p for the families of p -dependent two-qubit states indicated in the lower right panel. The dotted-line states are always separable and are nonzero discord QQ states for $p \neq 0, 1$, the dashed-line states (Werner states) are entangled for $p > 1/3$, whereas the solid-line states are entangled for $p \neq 1/2$. Above the threshold 1 (stars) the states are certainly entangled. (b) Same as previous for $|C_{AB}| + |C_{CD}|$, note that the QQ state (dotted line) is on the conjectured threshold 1 (stars) for this measure of correlation. (c) Same as previous for $S_{AB} + S_{CD}$. Here there are two entanglement boundaries: the states that have sum larger than 3 or smaller than 1 are conjectured to be entangled. Again, the dotted-state coincides with one of the conjectured boundaries. The dashed-line and the solid line are superimposed. Here $|\pm\rangle \equiv (|0\rangle \pm |1\rangle)/\sqrt{2}$ and $|\Phi^\pm\rangle \equiv (|00\rangle \pm |11\rangle)/\sqrt{2}$.

\mathcal{C}_{AB} , defined as

$$\mathcal{C}_{AB} \equiv \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle}{\sigma_A \sigma_B}, \quad (3)$$

where, as before, A and B denote observables relative to the two systems, $\langle X \rangle = \text{Tr}[X\rho]$ is the expectation value on the quantum state ρ and σ_X^2 is the variance of the observable X . The above quantity cannot be applied to eigenstates of A or B . Clearly, $\mathcal{C}_{AB} = 0$ for uncorrelated (product) states. In contrast to the classical Pearson correlation coefficient, the quantum one is, in general, complex if A and B do not commute, but as in the classical case, its modulus is upper-bounded by one:

$$|\langle AB \rangle - \langle A \rangle \langle B \rangle|^2 = \left| \frac{[A, B] + \{A, B\}}{2} - \langle A \rangle \langle B \rangle \right|^2 = \left| \frac{1}{2} [A, B] \right|^2 + \left| \frac{1}{2} \{A, B\} - \langle A \rangle \langle B \rangle \right|^2 \leq \sigma_A^2 \sigma_B^2, \quad (4)$$

where $[\cdot, \cdot]$ and $\{\cdot, \cdot\}$ denote the commutator and anti-commutator respectively, and where the final inequality

is the Schrödinger uncertainty relation [28].

We now use $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}|$ as a measure of complementary correlations to recover some entanglement properties of the system state. The Pearson coefficient gauges only the linear correlation of two stochastic variables, so it will not detect maximal correlation even for a maximally entangled state unless pairs of observables are linear in each others eigenvalues (e.g. it would fail if $A = \sum_j j|a_j\rangle\langle a_j|$ and $B = A^3$). However, if one restricts to linear observables, one can prove that a state is maximally entangled if and only if there exist two complementary bases such that $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 2$, e.g. if one uses $A = B = \sum_j j|a_j\rangle\langle a_j|$, $C = D = \sum_j j|c_j\rangle\langle c_j|$ where $|a_j\rangle$ and $|c_j\rangle$ are two complementary bases. The proof follows from the properties of the conditional probabilities (used to prove the analogous statement for the mutual information) and from the fact that the Pearson coefficient is ± 1 if and only if there is a functional relation that connects the two stochastic variables (details in supplemental material).

Instead, for non maximally entangled states we have two conjectures which are supported by numerical evidence: (i) If $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| > 1$, the two systems are entangled. As for the mutual information, the inequality is tight since ρ_{cc} is separable and has $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 1$; (ii) If $|\mathcal{C}_{AB}\mathcal{C}_{CD}| > 1/4$, the two systems are entangled. Also this inequality is tight: it is attained by the separable state $\sum_i (|a_i a_i\rangle\langle a_i a_i| + |c_i c_i\rangle\langle c_i c_i|)/2d$, with $|c_i\rangle$ eigenstates of C . As argued above, the conjecture with the product is weaker than the one with the sum: proving that all separable states have $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| \leq 1$ implies $|\mathcal{C}_{AB}\mathcal{C}_{CD}| \leq 1/4$.

The proof of these conjectures is complicated by the fact that the convexity properties of \mathcal{C}_{AB} are unknown. Nonetheless, they are natural conjectures that are easy to verify for large classes of states (e.g. see Fig. 2b). We have also performed extensive numerical checks by testing them on large sets of random states generated according to the prescription described in [29], and verifying that no state with non-positive partial transpose [3] lies over the conjectured threshold.

Note that the Pearson correlation only measures linear correlation, whereas the mutual information measures all types of correlations. So one could think that the latter is stronger and that these conjectures are implied by the mutual information results of the previous section. Surprisingly, this is false since there exist probability distributions that have maximal Pearson correlation but negligible mutual information [30]. Indeed, consider the family of entangled two-qubit states

$$|\psi_\epsilon\rangle = \epsilon|00\rangle + \sqrt{1-\epsilon^2}|11\rangle, \quad (5)$$

with $\epsilon \in [0, 1]$. If one uses $A = B = |1\rangle\langle 1|$ and $C = D = |+\rangle\langle +|$, for all $0 < \epsilon < 1$ such state has $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 1 + 2\epsilon\sqrt{1-\epsilon^2} > 1$ ([45]), but $|\psi_\epsilon\rangle$ clearly has negligible mutual information for $\epsilon \rightarrow 0$. In other

words, the Pearson correlation identifies $|\psi_\epsilon\rangle$ as entangled for all $0 < \epsilon < 1$ (assuming the above conjectures), whereas the mutual information does not even identify it as classically correlated *at all* for $\epsilon \rightarrow 0$. Indeed, numerical simulations suggest that Pearson correlation is more effective at detecting entanglement in random states than mutual information.

Sum of conditional probabilities:— The third measure of correlation we consider is the sum of conditional probabilities \mathcal{S}_{AB} , defined as

$$\mathcal{S}_{AB} \equiv \sum_i p(a_i|b_i), \quad (6)$$

where $p(a_i|b_i)$ is the probability of outcome a_i on the first system conditioned on result b_i on the second. [This is a somewhat limited measure of correlations as the correspondence $a_i \leftrightarrow b_i$ among results is clearly arbitrary. A more relevant measure of correlation should also maximize (or minimize) over the permutations of the measurement outcomes, but for the sake of simplicity we will avoid it.] In [17] a similar approach was used, but employing joint probabilities in place of conditional ones.

Gauging complementary correlations with the sum $\mathcal{S}_{AB} + \mathcal{S}_{CD}$ we can again obtain information about entanglement and quantum correlations: (i) Analogously to the case of the mutual information, the sum is optimized only for maximally entangled states: a state is maximally entangled if and only if there exist two complementary bases such that $\mathcal{S}_{AB} + \mathcal{S}_{CD} = 2d$; (ii) As for the Pearson correlation, we have a conjecture for non-maximally entangled states: if $\mathcal{S}_{AB} + \mathcal{S}_{CD}$ has a value outside the interval $[1, d+1]$, we conjecture that the two systems are entangled. As in the previous cases, the inequalities are tight since the upper bound is attained by the separable state ρ_{cc} and the lower bound by the separable state $\sum_i |a_i b_{i \oplus 1}\rangle\langle a_i b_{i \oplus 1}|/d$, with \oplus sum modulo d .

Let us analyse the case of separable states. We remind the reader that classical-quantum (CQ) and quantum-classical (QC) states have the form $\sum_i p_i |a_i\rangle\langle a_i| \otimes \rho_i$ and $\sum_i p_i \rho_i \otimes |a_i\rangle\langle a_i|$ respectively, where $\{|a_i\rangle\}$ is a set of orthogonal states for one subsystem and $\{\rho_i\}$ is not an orthogonal set of states. Note that separable quantum-quantum (QQ) states comprise all separable ones that are not CC, CQ or QC.

For these states we can prove that: (iii) if CC states have maximal correlations on one of two complementary variables, they are uncorrelated on the other [formally: if $p(a_i|b_i) = 1 \forall i$ then we must have $p(c_i|d_i) = 1/d \forall i$, where a_i, b_i, c_i, d_i are the results of the measurements of A, B, C, D with A complementary to C and B to D]; (iv) CQ states cannot have maximal correlations on any variable [formally: we cannot obtain $p(a_i|b_i) = 1 \forall i$, even when $p(c_i|d_i) = 1/d$]; (v) QQ states can have only *partial* correlation for each complementary property. For example, the separable two-qubit state $(|00\rangle\langle 00| + |11\rangle\langle 11| + |++\rangle\langle ++| + |--\rangle\langle --|)/4$

has partial correlation on both complementary variables, since $p(0|0) = p(1|1) = p(+|+) = p(-|-) = 3/4$.

Given the properties (iii) and (iv), one might suspect that separable states with non vanishing quantum correlations have always less complementary correlations, but this is not the case, as emphasized by (v). Summarizing, CC states can have maximal correlation only on one property, CQ states cannot have maximal correlation in any property, and QQ states can have some correlation on multiple properties, but you need pure, maximally entangled states to get maximal correlations on more than one property.

Regarding the result (i), the proof is a direct consequence of simple properties of conditional probabilities (see supplemental material) as for the cases seen previously. The difficulty in proving the conjecture (ii) stems again from a lack of definite concavity properties of \mathcal{S}_{AB} , but as for the previous conjecture we have extensively tested it numerically on random states. One may ask whether the sum over all outcomes in the statement of the conjecture is necessary. Indeed it is: the statement that all separable states satisfy $1/d \leq p(a_i|b_i) + p(c_i|d_i) \leq 1 + 1/d$ for some i is false (where the two bounds $1/d$ and $1 + 1/d$ give the bounds 1 and $d + 1$ we used above when the sum over i is performed). A counterexample is the separable state $(|00\rangle\langle 00| + |++\rangle\langle ++|)/2$ of two qubits for which $p(0|0) + p(+|+) = 5/3$. If one uses joint probabilities in place of conditional ones, a sufficient condition for entanglement can indeed be proven [17]. The results (iii) and (iv) can be proved at the same time by using simple properties of CC and CQ states when they are expressed in two complementary bases (see supplemental material), whereas property (v) is a direct consequence of the example provided above.

Extension to more complementary observables:— Up to now we have considered the correlations of the measurement outcomes of two complementary observables. All systems have at least three complementary observables [1], and it is known that there are $d + 1$ for d -dimensional systems if d is a power of a prime [1, 31]. Our results can be immediately extended to an arbitrary number of complementary observables by calculating the correlations of all the known complementary observables and considering the sum of the two largest ones. For example, for mutual information, we can extend the condition (1) to conclude that the state is entangled if

$$\max(I_{AB}, I_{CD}, I_{EF}, \dots) + \max_2(I_{AB}, I_{CD}, I_{EF}, \dots) > \log_2 d, \quad (7)$$

where \max_2 denotes the second largest term and where $A \otimes B$, $C \otimes D$, $E \otimes F$, etc. are all observables complementary to each other. The extensions of all other results and conjectures are analogous.

Moreover, at least in the case of qubits the bound at point (ii) for the mutual information and the conjectured

bound at point (i) for the Pearson correlations can be made stronger by adding correlations for the third complementary observable. This can improve significantly the efficiency of the present method if used for entanglement detection. For details and for a comparison with other known entanglement detection schemes based on measurements of MUBs see the supplemental material.

Conclusions:— In summary, we have introduced an interpretation of entanglement based on classical correlations of the measurement outcomes of complementary observables. We have studied different types of correlations (mutual information I , Pearson coefficient \mathcal{C} , and sum of conditional probabilities \mathcal{S}) for complementary observables of two systems. We have shown how they provide information on the entanglement and quantum correlations of a bipartite system. We have derived the following results and presented a few reasonable conjectures: (i) we proved necessary and sufficient conditions for maximal entanglement for I , \mathcal{C} , \mathcal{S} , (ii) we proved sufficient conditions for entanglement based on I and conjectured sufficient conditions based on \mathcal{C} and on \mathcal{S} ; (iii) when gauging complementary correlations using I , we proved that the separable states on the boundary with the entangled-states region are strictly classically correlated, but the same result is false if one uses \mathcal{C} or \mathcal{S} ; moreover we have shown how \mathcal{S} provides insight on CC, CQ, QC, and QQ states, showing that (iv) without entanglement only classically correlated CC states can have maximal correlation on one variable (but then they have no correlation on the complementary one), whereas (v) separable QQ states can have only partial correlations on complementary variables.

One can ask if it is possible to give necessary and sufficient conditions based on correlations for complementary observables. The naive statement that entangled states *always* have larger correlations than separable states is false, since it is known that entangled states exist (e.g. $|\psi_\epsilon\rangle$ defined above) that are arbitrarily close to separable pure states [32] and to the maximally mixed state (in the sense that for any distance ϵ one can choose a sufficiently large dimension d such that an entangled state is within distance ϵ from the maximally mixed state [33]). These have vanishing correlations for most measures of correlation. A notable exception, described above, is the Pearson coefficient that is able to detect the entanglement of $|\psi_\epsilon\rangle$ for all $\epsilon > 0$ (but it misses other types of entangled states).

We acknowledge useful feedback from B. Kraus, K. Życzkowski, and an anonymous Referee.

Supplemental Material. Proofs

Sufficient condition for entanglement using mutual information

Here we prove that if $I_{AB} + I_{CD} > \log_2 d$, then the state of the two systems is entangled. This theorem can equivalently be stated as: if the state is separable then $I_{AB} + I_{CD} \leq \log_2 d$.

The mutual information is

$$I_{AB} \equiv H(A) - H(A|B), \quad (8)$$

where $H(A)$ is the entropy of the A measurement outcomes and $H(A|B)$ is the conditional entropy of the A outcomes, which can be also written as

$$H(A|B) = - \sum_{a,b} p(a|b)p(b) \log_2 p(a|b) = \sum_b p(b) H(A|B=b), \quad (9)$$

where

$$H(A|B=b) = - \sum_a p(a|b) \log_2 p(a|b) \quad (10)$$

is the entropy of the probability distribution $p(a|b)$ for fixed b . By definition, separable states can be written as $\rho = \sum_l p_l \rho_l \otimes \sigma_l$. The conditional state $\rho^{(b)}$ when the result b is obtained from a B measurement on the second subsystem is

$$\rho^{(b)} = \sum_l \beta_l^{(b)} \rho_l, \quad \beta_l^{(b)} = p_l \langle b | \sigma_l | b \rangle / \sum_{l'} p_{l'} \langle b | \sigma_{l'} | b \rangle. \quad (11)$$

In the above expression for $\beta_l^{(b)}$ the term in the denominator is $p(b)$, namely the probability of getting outcome b when measuring B on the second subsystem. (Note that, in contrast to entangled states, the components ρ_l of the first subsystem have not changed, only the spectrum has changed.) The concavity of the entropy gives

$$H(A|B=b) = H(A)_{\rho^{(b)}} \geq \sum_l \beta_l^{(b)} H(A)_{\rho_l} \quad (12)$$

$$\Rightarrow H(A|B) = \sum_b p(b) H(A|B=b) \geq \sum_l p_l H(A)_{\rho_l},$$

where $H(X)_\rho$ denotes the Shannon entropy of a measurement of X on the state ρ . The same reasoning for C and D yields

$$H(C|D) \geq \sum_l p_l H(C)_{\rho_l}. \quad (13)$$

Now we use Maassen and Uffink's (MU) entropic uncertainty relation [27], which says that for any state ρ we have $H(A)_\rho + H(C)_\rho \geq -2 \ln c$ with $c = \max_{j,k} |\langle a_j | c_k \rangle|$.

For complementary observables, $-2 \ln c = \log_2 d$. This means that

$$H(A|B) + H(C|D) \geq \sum_l p_l [H(A)_{\rho_l} + H(C)_{\rho_l}] \geq \log_2 d, \quad (14)$$

where the first inequality is due to the concavity of the entropy, the second is the MU inequality. The above chain of inequalities and the fact that $H(A) \leq \log_2 d$, $H(C) \leq \log_2 d$ imply that

$$I_{AB} + I_{CD} = H(A) - H(A|B) + H(C) - H(C|D) \leq \log_2 d, \quad (15)$$

which concludes the proof.

Maximal mutual information for separable states

Here we prove that the separable states that satisfy $I_{AB} + I_{CD} = \log_2 d$, are classically-correlated (CC) zero-discord states.

The proof given in the previous section employs three inequalities: (a) the concavity of the entropy, (b) the MU inequality, and (c) the upper bounds for the entropy $H(A) \leq \log_2 d$ and $H(C) \leq \log_2 d$. We want now to find the states ρ for which the above three inequalities are equalities.

Inequality (b) is an equality only if ρ_l is a pure state and it is an eigenstate of either A or C [34]. We will first assume that all states ρ_l are eigenstates of A , namely $\rho_l = |a_l\rangle\langle a_l|$. Moreover, the conditions (c) become equalities iff the state of the first subsystem (obtained by tracing over the second) is $\mathbb{1}/d$. Therefore, in order to saturate the inequalities (b) and (c), the separable state must be of the form $\rho = \frac{1}{d} \sum_{l=0}^{d-1} |a_l\rangle\langle a_l| \otimes \sigma_l$, where $|a_l\rangle$ are eigenstates of A . Since the entropy is strictly concave, inequality (a) in Eq. (12) is saturated only if the states ρ_l for all l have the same entropy $H(A)_{\rho_l} = H(A)_{\rho^{(b)}}$ for the outcomes of measurements of A . Since the ρ_l s are all eigenstates of A , also $\rho^{(b)}$ must be an eigenstate of A , namely $\rho^{(b)} = |a_{l'}\rangle\langle a_{l'}|$ for some l' (i.e. $\beta_{l'}^{(b)} = \delta_{ll'}$). From the definition of $\beta_l^{(b)}$ in Eq. (11), this corresponds to σ_l being an eigenstate of B . Therefore, the form of the input state that fulfills the above requirements is

$$\rho_{cc} = \frac{1}{d} \sum_{l=0}^{d-1} |a_l\rangle\langle a_l| \otimes |b_l\rangle\langle b_l|. \quad (16)$$

For this state, Eq. (13) is then automatically satisfied with equality because we can write it as

$$\rho_{cc} = \frac{1}{d^2} \sum_l \sum_{jk} |c_j\rangle\langle c_k| e^{i[\theta(a_l, c_j) - \theta(a_l, c_k)]} \otimes |b_l\rangle\langle b_l| \quad (17)$$

$$= \frac{1}{d^2} \sum_j |c_j\rangle\langle c_j| \otimes \sum_l |b_l\rangle\langle b_l| + \sum_i \sum_{j \neq k} \dots, \quad (18)$$

where θ is some phase factor and where in the second line we have separated the part diagonal in c_j (which is the only one that contributes to the conditional probabilities) from the rest. In this form, it is clear that the probability distribution of the C measurement is uniform and independent of the outcome of the measurement D on the second subsystem. Therefore the concavity condition (a), see Eq. (13), gives again an equality. So, if ρ_l are all eigenstates of A , the state that satisfies (a), (b), and (c) with equality is the classically correlated state ρ_{cc} . The same argument *mutatis mutandis* applies to the case in which all ρ_l are eigenstates of C .

In order to complete the proof we have to exclude the case where both eigenstates of A and C appear in the input state ρ , namely a state of the form

$$p \sum_{l=0}^{d-1} p_l |a_l\rangle\langle a_l| \otimes \sigma_l + (1-p) \sum_{l=0}^{d-1} p'_l |c_l\rangle\langle c_l| \otimes \sigma'_l \quad (19)$$

(which, by an appropriate choice of p_l and p'_l may also describe states such as $(|a_0\rangle\langle a_0| \otimes \sigma_0 + |c_0\rangle\langle c_0| \otimes \sigma'_0)/2$). By taking the partial trace over the second subsystem and then multiplying to the left by $\langle a_m|$ and to the right by $|a_m\rangle$ for each m , one sees that this state cannot have identity as a marginal to saturate inequality (c) unless all terms in the first sum are nonzero. Analogously, using $\langle c_m|$ and $|c_m\rangle$ one sees that also all terms in the second sum are nonzero. Now, in order to saturate the concavity (a) of Eq. (12), all states ρ_l must have the same entropy for measurement of A as $\rho^{(b)}$ but, to saturate the MU inequality (b), it must also be equal to a pure state (either an eigenstate of A or of C). This is impossible for a state of the form (19) unless $p = 0$ or 1 , in which case we go back to the case considered above, that leads to the optimal states ρ_{cc} of (16).

Necessary and sufficient conditions for maximal entanglement

Here we prove the results on maximal entanglement. We start from the mutual information I and the sum of conditional probabilities \mathcal{S} . The case of the Pearson coefficient is treated separately below.

Start by proving that if $I_{AB} + I_{CD} = 2 \log_2 d$ or $\mathcal{S}_{AB} + \mathcal{S}_{CD} = 2d$ then the state is maximally entangled (the converse will be proven below). From the definition of I_{AB} in Eq. (8), it is upper bounded by $\log_2 d$ and can achieve this bound only when the conditional entropy is null. Since the conditional entropy is defined as

$$H(A|B) \equiv - \sum_{a,b} p(a,b) \log_2 p(a|b), \quad (20)$$

it is null only when the conditional probabilities are 0 or 1 which implies the result for $\mathcal{S}_{AB} + \mathcal{S}_{CD}$. We first prove this for two qubits for simplicity, with the two

complementary properties identified by projectors on the computational basis $\{|0\rangle, |1\rangle\}$ and on the Fourier basis $\{|\pm\rangle = |0\rangle \pm |1\rangle\}$. We prove that if $p(0|0) = p(1|1) = p(+|+) = p(-|-) = 1$, the state of the two systems is a maximally entangled state $|\Psi^+\rangle$. The conditional probability is $p(0|0) = \text{Tr}[|0\rangle\langle 0| \rho_0]$, where ρ_0 is the state conditioned on obtaining 0 on the second system:

$$\rho_0 = \frac{{}_B\langle 0|\rho|0\rangle_B}{\text{Tr}[{}_B\langle 0|\rho|0\rangle_B]} \Rightarrow p(0|0) = \frac{\langle 00|\rho|00\rangle}{\langle 00|\rho|00\rangle + \langle 10|\rho|10\rangle} \quad (21)$$

where ρ is the initial state of the composite system. From the above expression we have that $p(0|0) = 1$ only if $\langle 10|\rho|10\rangle = 0$. By the same argument for $p(1|1)$ we can conclude that $\langle 01|\rho|01\rangle = 0$, so that ρ must belong to the subspace spanned by $\{|00\rangle, |11\rangle\}$. Note that $\langle 10|\rho|10\rangle = \langle 01|\rho|01\rangle = 0$ implies that also $\langle 10|\rho|01\rangle + \langle 10|\rho|01\rangle = 0$ (see below). This means that

$$\begin{aligned} \langle ++|\rho|++\rangle &= \langle 00|\rho|00\rangle + \langle 11|\rho|11\rangle + \langle 00|\rho|11\rangle + \langle 11|\rho|00\rangle \\ \langle -+|\rho|-+\rangle &= \langle 00|\rho|00\rangle + \langle 11|\rho|11\rangle - \langle 00|\rho|11\rangle - \langle 11|\rho|00\rangle \\ \Rightarrow p(+|+) &= \frac{\langle 00|\rho|00\rangle + \langle 11|\rho|11\rangle + \langle 00|\rho|11\rangle + \langle 11|\rho|00\rangle}{2(\langle 00|\rho|00\rangle + \langle 11|\rho|11\rangle)}, \end{aligned}$$

which is $p(+|+) = 1$ if and only if $\langle 00|\rho|00\rangle + \langle 11|\rho|11\rangle = \langle 00|\rho|11\rangle + \langle 11|\rho|00\rangle$. The above relation holds if and only if ρ is a pure state, and is equal to $\rho = |\Psi^+\rangle\langle\Psi^+|$.

In order to prove this we employ the inequality $\rho_{nn} + \rho_{mm} \geq \rho_{nm} + \rho_{mn}$ which is an equality only for states that are pure and balanced when restricted to the $\{|m\rangle, |n\rangle\}$ subspace, namely for states that in such subspace are $|m\rangle + |n\rangle$. This inequality can be easily proved by decomposing $\rho = \sum_i \lambda_i |i\rangle\langle i|$ and using the same inequality for pure states: $|\alpha|^2 + |\beta|^2 \geq \alpha^* \beta + \beta^* \alpha$ (where $\alpha = \langle n|\psi\rangle$, $\beta = \langle m|\psi\rangle$), which can be easily derived noticing that $0 \leq |\alpha - \beta|^2 = |\alpha|^2 + |\beta|^2 - \alpha^* \beta - \beta^* \alpha$, where equality holds if and only if $\alpha = \beta$.

We will now extend the above proof to couples of systems in arbitrary finite dimension d . The matrix elements of the global state ρ in the computational basis are denoted for brevity as $\langle ij|\rho|kl\rangle = \rho_{ij,kl}$. The conditions that the conditional probabilities in the computational basis must be one are given by

$$p(0|0) = \frac{\rho_{00,00}}{\sum_{i=0}^{d-1} \rho_{i0,i0}} = 1. \quad (22)$$

The above condition is satisfied iff $\sum_{i=1}^{d-1} \rho_{i0,i0} = 0$, which implies that $\rho_{i0,i0} = 0$ for $i \neq 0$. The same argument holds for the conditional probability $p(j|j)$ and we then have

$$p(j|j) = \frac{\rho_{jj,jj}}{\sum_{i=0}^{d-1} \rho_{ij,ij}} = 1. \quad (23)$$

The above condition is satisfied iff $\sum_{i \neq j}^{d-1} \rho_{ij,ij} = 0$ for fixed j , which implies that $\rho_{ij,ij} = 0$ for $i \neq j$. As a

consequence, the positivity of ρ requires that $\rho_{ij,kl} = 0$ for $i \neq j, k \neq l$. The above conditions then imply that the only nonvanishing elements of ρ are of the form $\rho_{ii,jj}$.

Let us now denote as $\{|\bar{j}\rangle, j = 0, d-1\}$ the Fourier transform of the computational basis, namely

$$|\bar{j}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{i2\pi kj/d} |k\rangle. \quad (24)$$

The matrix elements in the Fourier transformed basis can be written as

$$\begin{aligned} \rho_{\bar{0}\bar{0},\bar{0}\bar{0}} &= \frac{1}{d^2} \sum_{j,k=0}^{d-1} \rho_{jj,kk} \\ \rho_{\bar{j}\bar{0},\bar{j}\bar{0}} &= \frac{1}{d^2} \sum_{j,k=0}^{d-1} e^{i2\pi(k-j)\bar{j}/d} \rho_{jj,kk}. \end{aligned} \quad (25)$$

The conditional probability $p(\bar{0}|\bar{0})$ then takes the form

$$p(\bar{0}|\bar{0}) = \frac{\sum_{j,k=0}^{d-1} \rho_{jj,kk}}{\sum_{\bar{i}=0}^{d-1} \sum_{j,k=0}^{d-1} e^{i2\pi(k-j)\bar{i}/d} \rho_{jj,kk}}. \quad (26)$$

By using the identity

$$\sum_{\bar{i}=0}^{d-1} e^{i2\pi l\bar{i}/d} = d\delta_{l,kd}, \quad (27)$$

which means that the l.h.s. of Eq. (27) vanishes for all values of l that are not multiples of the dimension d , we can write the denominator in Eq. (26) as

$$\sum_{j,k=0}^{d-1} \rho_{jj,kk} \sum_{\bar{i}=0}^{d-1} e^{i2\pi(k-j)\bar{i}/d} = d \sum_{j=0}^{d-1} \rho_{jj,jj}, \quad (28)$$

By imposing that the probability in Eq. (26) must be one we have that

$$p(\bar{0}|\bar{0}) = \frac{\sum_{j,k=0}^{d-1} \rho_{jj,kk}}{d \sum_{j=0}^{d-1} \rho_{jj,jj}} = 1. \quad (29)$$

By the same reasoning as for the qubit case the above condition implies that ρ is a projector onto the maximally entangled state $|\Phi^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |jj\rangle$.

To finish the proof for I and \mathcal{S} , we have to prove the converses: if the state is maximally entangled, then there exist two complementary bases such that $I_{AB} + I_{CD} = 2\log_2 d$ or $\mathcal{S}_{AB} + \mathcal{S}_{CD} = 2d$. Any maximally entangled state $|\Psi\rangle$ is local-unitarily equivalent to $|\Phi^+\rangle \equiv \sum_j |jj\rangle/\sqrt{d}$. Namely, $|\Psi\rangle = U \otimes U' |\Phi^+\rangle$ with U and U' unitaries (which transform local bases one into another). The same result as for $|\Phi^+\rangle$ can then be achieved by starting from $|\psi\rangle$ and considering as complementary bases the ones that are obtained by applying $U^\dagger \otimes U'^\dagger$ to the computational and the Fourier bases.

Finally, to prove the necessary and sufficient condition for the Pearson coefficient \mathcal{C} , we note that we have just shown that a state has maximal correlation for two complementary bases if and only if it is local-unitarily equivalent to $|\Phi^+\rangle$. Namely, in two complementary bases, the local outcomes match: $\mathcal{S}_{AB} + \mathcal{S}_{CD} = 2d$. It is known that the Pearson coefficient takes its extremal values ± 1 iff the two stochastic variables are linearly dependent and perfectly correlated (i.e. in one-to-one correspondence).

Sum of conditional probabilities for CC and CQ states

Here we prove that CC states can have maximal correlations only on one of two complementary variables and that CQ states cannot have maximal correlations on any variable. The first statement is formalized above as: if $p(a_i|b_i) = 1 \forall i$ then we must have $p(c_i|d_i) = 1/d \forall i$, where a_i, b_i, c_i, d_i are the results of the measurements of A, B, C, D . The second statement is formalized as: even if $p(c_i|d_i) = 1/d \forall i$ we still cannot obtain $p(a_i|b_i) = 1 \forall i$.

We can prove both statements at the same time by observing that CC and CQ states can be written in the form

$$\rho_d = \sum_a p_a |a\rangle\langle a| \otimes \rho_a,$$

which can have maximal correlation on some property only for CC states (where the ρ_a are orthogonal for different a). We can then show that the state ρ_d which has some correlation on a cannot have any correlation on c when c is a complementary property, namely if $|\langle c|a\rangle|^2 = 1/d$. Actually,

$$\rho_d = \sum_a \sum_{c,c'} \frac{p_a}{d} |c\rangle\langle c'| e^{i[\theta(a,c) - \theta(a,c')]} \otimes \rho_a \quad (30)$$

$$= \sum_c \frac{1}{d} |c\rangle\langle c| \otimes \sum_a p_a \rho_a + \sum_a \sum_{c \neq c'} \dots, \quad (31)$$

where θ is some phase factor and where, as above, in the second line we have separated the part diagonal in c (which is the only one that contributes to the correlations for c) from the rest. It is clear from the form of the state in (31) that such a state does not have any correlations in c : namely that a measurement of C on the first system gives no information on the second.

Correlations on 3 MUBs for qubits

Following a suggestion by an anonymous referee, we prove here that the sufficient condition $I_{AB} + I_{CD} > 1$ for entanglement of pairs of qubits can be made stronger by adding a third MUB for each qubit, which we name E and F . Actually, for a separable two-qubit state the

argument given in the first supplemental section until Eq. (13) can be applied also for the third pair of bases EF . We can then write

$$H(A|B) + H(C|D) + H(E|F) \geq \sum_l p_l [H(A)_{\rho_l} + H(C)_{\rho_l} + H(E)_{\rho_l}]. \quad (32)$$

We can then exploit a generalisation of the MU inequality to the case of three MUBs A, C, E for qubits provided in [35], which says that for any qubit state ρ we have $H(A)_\rho + H(C)_\rho + H(E)_\rho \geq 2$. We can then conclude that separable states fulfill the condition

$$I_{AB} + I_{CD} + I_{EF} \leq 1. \quad (33)$$

The conjectured bound

$$C_{AB} + C_{CD} \leq 1 \quad (34)$$

for separability in terms of Pearson correlations can also be extended to three MUBs, leading to

$$C_{AB} + C_{CD} + C_{EF} \leq 1. \quad (35)$$

The latter has been tested numerically (see also the next section). In Fig. 3 we report the corresponding results for the mutual information and the Pearson correlations with three MUBs, to be compared with Fig. 2, where only two MUBs are considered. As we can see, the improvement is striking. In particular note that the Pearson correlations are now suitable to detect all Werner states since they signature the presence of entanglement for $p > 1/3$.

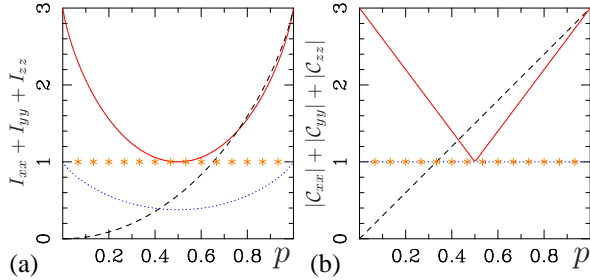


FIG. 3: Extension of Fig. 2 to the case in which three complementary observables are used for a qubit. (a) Sum of the mutual information $I_{xx} + I_{yy} + I_{zz}$ plotted as a function of p for the same families of states presented in Fig. 2. Note how the criterion now detects a larger portion of the Werner states as entangled. The stars indicate the threshold above which the states are entangled. (b) Sum of the Pearson correlation coefficients $|C_{xx}| + |C_{yy}| + |C_{zz}|$ plotted as a function of p . The stars indicate the conjectured threshold above which states should be entangled. Note that all the entangled Werner states (i.e. the ones for $p > 1/3$) are above the conjectured threshold: all entangled Werner states are identified by the Pearson correlation.

Comparison of entanglement detection methods

In this section we study the effectiveness of our entanglement criterion based on complementary correlations to detect entanglement and compare it to known entanglement detection schemes. We stress that our proposal is not aimed at introducing a new entanglement detection scheme but it is aimed at giving a new interpretation of entanglement in terms of correlations for complementary properties. Nonetheless, interestingly we see that these perform better than entanglement witnesses that employ the same measurements. Moreover, entanglement detection based on correlations for complementary properties allows to detect many entangled states that entanglement witnesses miss.

In the following we provide a comparison between our method and an entanglement detection scheme based on the use of witness operators [36]. For simplicity, we compare the case of two qubit states, where entanglement witnesses that involve measurements of three complementary properties of qubits take a simple form, namely

$$W_1 = (\mathbb{1} + \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)/4 \quad (36)$$

$$W_2 = (\mathbb{1} - \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)/4 \quad (37)$$

$$W_3 = (\mathbb{1} + \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)/4 \quad (38)$$

$$W_4 = (\mathbb{1} + \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y - \sigma_z \otimes \sigma_z)/4 \quad (39)$$

$$W_5 = (\mathbb{1} - \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y - \sigma_z \otimes \sigma_z)/4. \quad (40)$$

If $\text{Tr}[\rho W_i] < 0$ for at least one of $i = 1, \dots, 5$ for a two-qubit state ρ , then the state is entangled. The first four operators are witness operators optimised for the Bell states [37], while W_5 was added in order to include also the detection scheme based on the inequality $-1 \leq \langle \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z \rangle \leq 1$ for separable states [16]. Actually, testing for W_1 and W_5 allows to test the above condition. We performed a comparison between these detection schemes and our criterion (extended to all three complementary bases of qubits as shown in the previous section) with a Monte Carlo simulation, by considering 10^8 random states obtained by generating 4×4 random matrices according to the method detailed in [38, 39]. Whether each state is entangled or not can be evaluated with the PPT criterion [3], which is a necessary and sufficient condition in this case: we found that 36.87% of the states are entangled, which is consistent with known results [38]. The Pearson coefficient conjecture detects 9.67% of these entangled states, whereas the entanglement witnesses detect 8.61% of them. Therefore, the Pearson coefficient turns out to be more powerful for entanglement detection.

In Fig. 4a and the first panel of table I we compare the performance of these witnesses against the Pearson correlation conjecture. Note that 24.48% of the detected entangled states are not detected by the entanglement witnesses and are seen only by the Pearson coefficient

conjecture (this corresponds to a fraction 28.88% of the entangled states detected using the Pearson coefficient: these are detected only by the Pearson correlations). The entanglement witnesses are less effective: they exclusively detect 15.23% of the detected states (this corresponds to a fraction 20.17% of the states detected by the entanglement witnesses). In Fig. 4b and the second panel of table I we compare also the performance of the sum of conditional probabilities conjecture. The mutual information does not perform well for entanglement detection, but interestingly most of the (few) entangled states it detects are distinct from the ones detected by the witnesses, as seen from the third panel in table I.

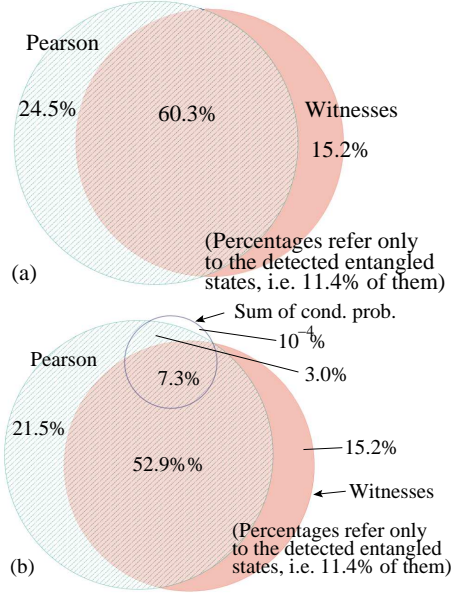


FIG. 4: Venn diagrams [40] to compare the efficiency of different entanglement detection schemes. (a) Comparison between the entanglement witnesses and the Pearson coefficient conjecture. (b) Comparison between the entanglement witnesses, the Pearson coefficient conjecture and the sum of conditional probabilities.

We now present a comparison between the Pearson conjecture and a relation (proposed by an anonymous Referee) based on local uncertainty relations (LUR) [5] for qubits. Indeed the LUR implies that all separable states have $\Delta^2(\sigma_x \otimes \mathbb{1} - \mathbb{1} \otimes \sigma_x) + \Delta^2(\sigma_z \otimes \mathbb{1} - \mathbb{1} \otimes \sigma_z) \geq 2$. This is obtained from the uncertainty relation $\Delta^2(\sigma_x) + \Delta^2(\sigma_z) \geq 1$. This condition is equivalent to saying that all separable states satisfy

$$|C'_{XX}| + |C'_{ZZ}| \leq (\Delta_{\rho_1}^2(\sigma_x) + \Delta_{\rho_2}^2(\sigma_x) + \Delta_{\rho_1}^2(\sigma_z) + \Delta_{\rho_2}^2(\sigma_z))/2 - 1, \quad (41)$$

where ρ_1 is the reduced state over the first subsystem and ρ_2 over the second, and where $C'_{AB} = \langle AB \rangle - \langle A \rangle \langle B \rangle$. The comparison between this entanglement detection condition and the Pearson conjecture is presented in

Detection scheme	Entangled states detected
only witness	15.23%
only Pearson	24.48%
both	60.29%
only witness	15.23%
only Pearson	21.51%
only cond. prob.	0.0%
only witness and Pearson	52.95%
only witness and cond. prob.	0.0%
only Pearson and cond. prob.	2.98%
all	7.34%
only witness	15.23%
only Pearson	24.48%
only mutual info	0.0%
only cond. prob.	0.0%
only witness and Pearson	52.95%
only witness and mutual info	0.0%
only witness and cond. prob.	0.0%
only Pearson and mutual info	0.0%
only Pearson and cond. prob.	2.78%
only mutual info and cond. prob.	0.0%
witness, Pearson, mutual info	0.001%
witness, Pearson, cond. prob.	6.72%
witness, mutual info, cond. prob.	0.0%
Pearson, mutual info, cond. prob.	0.2%
all	0.61%

TABLE I: Monte Carlo simulation results. The first panel compares the witnesses W_1, \dots, W_5 with the Pearson conjecture, the second panel adds also the sum of conditional probabilities conjecture, the third panel adds the mutual information. The first two tables are graphically depicted in Fig. 4. The percentages depicted refer to the fraction of the entangled states that were detected by at least one of the methods, which is a fraction of 11.41% of the entangled states in all cases since the mutual information and the sum of conditional entropies detect very few new entangled states that are not detected by the other two schemes: on the order of $10^{-4}\%$). We sampled 10^8 random 4×4 states and interpreted them as two-qubit states.

Fig. 5, whence it is evident that the Pearson conjecture (35) that uses three complementary observables identifies many more entangled states than (41), which can identify only very few states (0.39% of the identified ones) that are not seen by the Pearson conjecture. If one, instead, limits the Pearson conjecture to the same two complementary observables employed in (41) as in (34), then the former procedure results stronger, as it identifies all the entangled states seen.

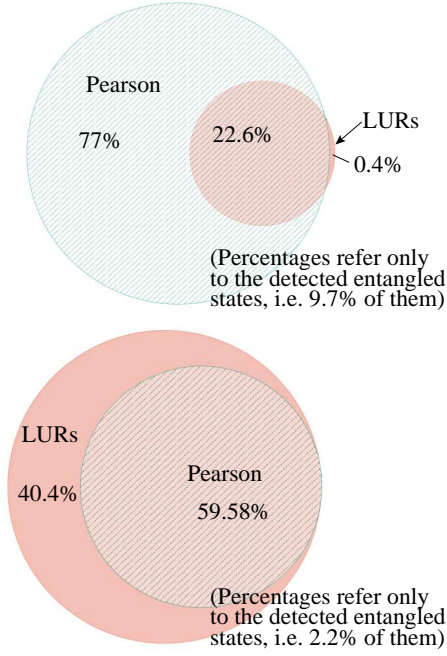


FIG. 5: Venn diagram [40] to compare the efficiency of the Pearson correlation conjecture and the condition (41) based on local uncertainty relations (LURs). The data has been obtained from a Monte Carlo simulation of 10^8 random matrices. The figure above refers to the Pearson conjecture with three complementary observables (35), the figure below to the Pearson conjecture with two (34).

Efficiency of complementary correlations as entanglement criterion

We want to discuss here the efficiency of our proposal as an entanglement criterion. It is clear from our proof above that our criterion could be immediately strengthened by considering just the entropic uncertainty relations [10] instead of considering the mutual information: in fact, inequality (14) is clearly stronger than (15). A discussion on these grounds goes beyond our aims: we do not want to provide a strong entanglement criterion, but a different way to interpret entanglement. Nonetheless, the question of how strong is our proposal as entanglement criterion is a relevant one and we will explore it in this section.

Let us first distinguish between entanglement detection and entanglement criteria. The first refers to a measurement procedure, whose aim is to determine whether a given state is entangled or not using measurements that are independent of the state. The second refers to a general characterization of entanglement: how well does some criterion (in our case, the classical correlation among complementary observables) characterize entanglement?

It turns out that our proposal is quite effective in characterizing entanglement. For low dimensions, we explore

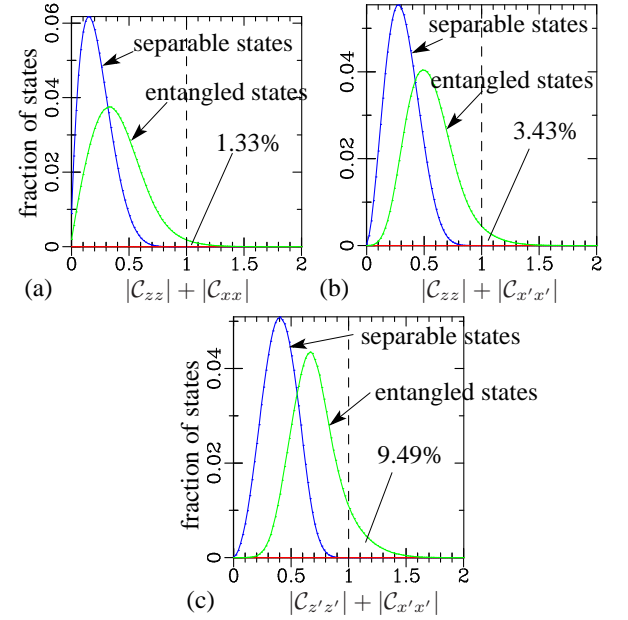


FIG. 6: Our method seen as an entanglement criterion: effect of the optimization over the complementary observables (only two, σ_x and σ_z , of the three complementary observables of the qubit are optimized here). (a) Distribution of the Pearson correlation $|C_{zz}| + |C_{xx}|$ for 10^8 randomly generated states without optimization. Only 1.33% of the entangled states are above the threshold $|C_{zz}| + |C_{xx}| = 1$ (vertical dashed line), and are detected as entangled without any optimization. (b) Same as previous, but optimizing the second observable among 80 different directions of the Fourier basis (using the same basis for the two qubits). Compared with the previous case, note how the optimization reduces the overlap between the separable (blue or dark grey) and entangled (green or light grey) distributions pushing the entangled distribution over the threshold. Now a percentage 3.43% of entangled states are detected as such. Here 10^8 random states have been employed. (c) Double optimization over the two bases (for 40 values of the Fourier basis for each of 40 different choices of computational basis). The overlap among the histograms is further reduced and now a percentage of 9.49% states are detected as entangled. Here 10^7 random states have been employed. A further increase in efficiency would be achieved by optimizing over all three complementary observables of a qubit, and for different directions for each of the two qubits: see Fig. 7.

this numerically for mixed states. In Fig. 6 we explore numerically the use of the Pearson coefficient conjecture as an entanglement criterion by using only two MUBs and by optimizing the complementary observables for each entangled state. For qubits, optimizing only over the second observable already yields an increase in the detected states: one goes from a fraction 1.33% of detected entangled states up to 3.43%. An optimization over both observables achieves a further increase up to a fraction 9.49% of entangled states detected.

Note that the first number 1.33% is lower than the one reported in the previous section, where we reported that

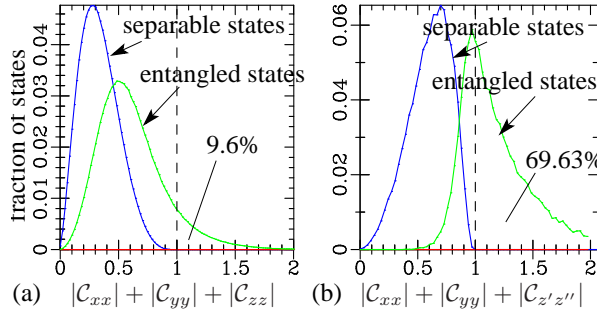


FIG. 7: Same as Fig. 6, but where all three different complementary observables of the two qubits have been considered. (a) Distribution of the Pearson correlation $|C_{xx}| + |C_{yy}| + |C_{zz}|$ for 10^7 randomly generated states without optimization. Here 9.65% of the entangled states are above the threshold $|C_{xx}| + |C_{yy}| + |C_{zz}| = 1$ (vertical dashed line), and are detected as entangled without any optimization, consistently with the results presented in the previous section (Fig. 4, where $84.8\% = 60.3\% + 24.5\%$ of 11.4% gives indeed 9.66%). (b) Same as previous, but optimizing one observable among 10^5 different directions chosen randomly with uniform probability (and independently for each qubit). Compared with the previous case, note how the optimization reduces the overlap between the separable (blue or dark grey) and entangled (green or light grey) distributions pushing the entangled distribution over the threshold. Now a percentage 69.63% of entangled states are detected as such. Here 10^5 random states have been employed.

the Pearson correlation detects a much larger fraction of the entangled states, namely $84.8\% = 60.3\% + 24.5\%$ of the detected entangled states which are 11.4% of the total states, namely $9.7\% = .848 \times .114$ of the total states are detected as entangled. The reason that we achieve only 1.33% here is because we only considered two instead of the three complementary observables of a qubit: that optimization would lead to the increase $1.33\% \rightarrow 9.7\%$, as shown in Fig. 7a.

As mentioned above, in these simulations we have only considered two complementary observables (σ_z and σ_x). Further increases can be achieved if one optimizes over all three complementary observables of qubits: see Fig. 7. As regards to the percentage given in Fig. 7b, we have to note one should be able to further increase it by optimizing also over all three complementary observables, instead of only one. Preliminary investigations in this direction are promising but numerically very demanding. It is difficult to provide an estimate of the statistical error since the fluctuations due to the Monte Carlo simulations are non Gaussian in this case.

Finally, we mention that our method becomes almost an optimal criterion for large dimensions and pure states according to an argument pointed out by K. Życzkowski [41]. Unfortunately it is practically impossible to explore numerically this regime. Życzkowski's argument [41] is based on the fact that for $d \rightarrow \infty$ almost all pure entangled states are close to maximally entangled, since the

average entanglement of randomly chosen d -dimensional pure states goes as $\ln d - 1/2 + O(\ln d/d)$ [42]. For large d , the term $1/2$ becomes irrelevant. Since our criterion gives a necessary-and-sufficient condition for maximally entangled states, it will then asymptotically detect almost all pure entangled states for $d \rightarrow \infty$. This is only a heuristic argument, however: one must account for the fact that the convergence to maximal entanglement might be so slow that the above argument might only be meaningful in the limit $d \rightarrow \infty$. In this regime our proof (valid for finite d) does not hold, and discontinuities might be present [43].

-
- [1] T. Durt, B.-G. Englert, I. Bengtsson, K. Życzkowski, *Int. J. Quantum Information* **8**, 535 (2010).
 - [2] D. Bruß, *J. Math. Phys.* **43**, 4237 (2002); R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki, *Rev. Mod. Phys.* **81**, 865 (2009).
 - [3] A. Peres, *Phys. Rev. Lett.* **77**, 1413 (1996); M. Horodecki, P. Horodecki, R. Horodecki, *Phys. Lett. A* **223**, 1 (1996).
 - [4] G. Vidal, R.F. Werner, *Phys. Rev. A* **65**, 032314 (2002).
 - [5] H.F. Hofmann, S. Takeuchi, *Phys. Rev. A* **68**, 032103 (2003).
 - [6] J. Schlienz and G. Mahler, *Phys. Rev. A* **52**, 4396 (1995).
 - [7] C. Kothe, G. Björk, *Phys. Rev. A* **75**, 012336 (2007); I.S. Abascal, G. Björk, *Phys. Rev. A* **75**, 062317 (2007).
 - [8] O. Gühne, M. Mechler, G. Tóth, P. Adam, *Phys. Rev. A* **74**, 010301(R) (2006).
 - [9] C.-J. Zhang, Y.-S. Zhang, S. Zhang, G.-C. Guo, *Phys. Rev. A* **76**, 012334 (2007).
 - [10] V. Giovannetti, *Phys. Rev. A* **70**, 012102 (2004).
 - [11] O. Gühne and M. Lewenstein, *Phys. Rev. A* **70**, 022316 (2004).
 - [12] Y. Huang, *Phys. Rev. A* **82**, 012335 (2010).
 - [13] P.J. Coles, M. Piani, *Phys. Rev. A* **89**, 022112 (2014); P.J. Coles, *Phys. Rev. A* **85**, 042103 (2012).
 - [14] B.M. Terhal, *Linear Algebra Appl.* **323**, 61 (2000), arXiv:quant-ph/9810091; O. Gühne, G. Tóth, *Physics Reports* **474**, 1 (2009).
 - [15] M. Lewenstein, B. Kraus, J.I. Cirac, P. Horodecki, *Phys. Rev. A* **62**, 052310 (2000).
 - [16] G. Tóth, *Phys. Rev. A* **71**, 010301(R) (2005); M.R. Dowling, A.C. Doherty, S.D. Bartlett, *Phys. Rev. A* **70**, 062113 (2004).
 - [17] C. Spengler, M. Huber, S. Brierley, T. Adaktylos, B.C. Hiesmayr, *Phys. Rev. A* **86**, 022311 (2012); B.C. Hiesmayr, W. Löffler, *New J. Phys.* **15**, 083036 (2013).
 - [18] W.K. Wootters, *Phys. Rev. Lett.* **80**, 2245 (1998).
 - [19] O. Rudolph, *Quantum Inf. Process.* **4**, 219 (2005), arXiv:quant-ph/0202121.
 - [20] O. Gühne, *Phys. Rev. Lett.* **92**, 117903 (2004).
 - [21] J.I. de Vicente, *Quantum Inf. Comput.* **7**, 624 (2007); J.I. de Vicente, M. Huber, *Phys. Rev. A* **84**, 062306 (2011).
 - [22] O. Gühne, P. Hyllus, O. Gittsovich, J. Eisert, *Phys. Rev. Lett.* **99**, 130504 (2007).
 - [23] O. Gittsovich, O. Gühne, P. Hyllus, J. Eisert, *Phys. Rev. A* **78**, 052319 (2008).
 - [24] C.-J. Zhang, Y.-S. Zhang, S. Zhang and G.-C. Guo, *Phys. Rev. A* **77**, 060301(R) (2008).

- [25] S. Wu, Z. Ma, Z. Chen, S. Yu, Sci. Rep. **4**, 4036 (2014).
- [26] J. Schneeloch, C.J. Broadbent, S.P. Walborn, E.G. Cavalcanti, J.C. Howell, Phys. Rev. A **87**, 062103 (2013); J. Schneeloch, C.J. Broadbent, J.C. Howell Phys. Rev. A **90**, 062119 (2014).
- [27] H. Maassen, J.B.M. Uffink, Phys. Rev. Lett. **60**, 1103 (1988).
- [28] E. Schrödinger, Sitzungsberichte der Preussischen Akademie der Wissenschaften, Physikalisch-Mathematische Klasse 14: **296**, 303 (1930).
- [29] K. Życzkowski, P. Horodecki, A. Sanpera, M. Lewenstein, Phys. Rev. A **58**, 883 (1998).
- [30] D.V. Foster, P. Grassberger, Phys. Rev. E **83**, 010101(R) (2011).
- [31] W. K. Wootters, B. D. Fields, Ann. Phys. **191**, 363 (1989).
- [32] M.A. Nielsen, J. Kempe, Phys. Rev. Lett. **86**, 5184 (2001).
- [33] A.O. Pittenger, M.H. Rubin, Phys. Rev. A **62**, 032313 (2000).
- [34] A.R. Gonzales, J.A. Vaccaro and S.M. Barnett, Phys. Lett. A **205**, 247 (1995).
- [35] J. Sanchez, Phys. Lett. A **173**, 233 (1993).
- [36] O. Gühne, P. Hyllus, D. Bruß, A. Ekert, M. Lewenstein, C. Macchiavello and A. Sanpera, Phys. Rev. A **66**, 062305 (2002).
- [37] O. Gühne, P. Hyllus, D. Bruß, A. Ekert, M. Lewenstein, C. Macchiavello and A. Sanpera, J. Mod. Opt. **50**, 1079 (2003).
- [38] K. Życzkowski, P. Horodecki, A. Sanpera, M. Lewenstein, Phys. Rev. A **58**, 883 (1998).
- [39] M. Pozniak, K. Życzkowski, M. Kus, J. Phys. A: Math. Gen. **31**, 1059 (1998).
- [40] The Venn diagrams are plotted with the app presented in L. Micallef, P. Rodgers PLoS ONE **9**, e101717 (2014), <http://www.eulardiagrams.org/eulerAPE>.
- [41] K. Życzkowski, Private communication (during a memorable hike in the Iranian mountains) (2014).
- [42] K. Życzkowski, H.-J. Sommers, J. Phys. A: Math. Gen. **34**, 7111 (2001),
- [43] J. Eisert, C. Simon, M.B. Plenio, J. Phys. A: Math. Gen. **35**, 3911 (2002).
- [44] Many results can be immediately extended to the case where the two systems have different dimensions.
- [45] In accordance to the result for maximally entangled states, the sum is equal to 2 only for the maximal entangled state $|\Phi^+\rangle = |\psi_{\epsilon=1/\sqrt{2}}\rangle$.